Physics 220: Final Project
due June 2, 2011.

Consider the 2d Ising model, $H = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j$, where $\sigma_i = \pm 1$ and $J = 1$. You can use whatever programming language you like: C, C++, fortran, python, matlab, even mathematica. Your final report should include your program, emailed to me, and a written summary of your calculations and answers to the questions below. Answer Part 1 completely. Choose *one* of the remaining parts.

1. Write a Monte Carlo simulation for the model on the square lattice of $N = L \times L$ sites with periodic boundary conditions using the Metropolis algorithm. Start from a random initial state, and choose subsequent states as follows:

   - Choose the next trial configuration by randomly flipping one spin.
   - Calculate the energy difference, ΔE, between the trial state and the old state.
   - If $\Delta E < 0$, accept the new state as the next one. If $\Delta E > 0$, generate a random number $0 \leq r < 1$, and accept the trial state if and only if $e^{-\beta\Delta E} > r$.

   Thermal averages can be estimated by averages over samples, $\langle\mathcal{O}\rangle = \frac{1}{M}\sum_{i=1}^{M}\mathcal{O}_i$, where the sum is over M samples i.

   (a) Plot the average energy $\langle E\rangle/N$ per site for $L = 16$ at $\beta = 1$ and $\beta = 3$, as a function of the Monte Carlo step i. You should see an initial period in which the energy changes rapidly, before fluctuating around equilibrium. Data during this "warm up" period should not be used in the thermodynamic averages calculated below.

   (b) Plot the average energy per site versus temperature. Average over at least 10^5 Monte Carlo steps per temperature. Plot the (absolute value of) the average magnetization per site $|\langle M\rangle|/N$ and the square root of the variance of the same quantity, $\langle M^2\rangle/N^2$, versus temperature. Discuss the behavior at $T \to 0$ and $T \to \infty$.

   (c) Show (analytically) that the specific heat is given by $c_v = \left(\langle E^2\rangle - \langle E\rangle^2\right)/(NT^2)$. Calculate this using Monte Carlo and plot it versus temperature to obtain a rough estimate of T_c.

   (d) The magnetic susceptibility is similarly given by $\chi = \left(\langle M^2\rangle - \langle M\rangle^2\right)/(NT)$. Plot χ versus T for $L = 8, 12, 16$, and 20. Do the same for the quantity $\chi' = \left(\langle M^2\rangle - \langle|M|\rangle^2\right)/(NT)$. How similar are both quantities?

   (e) By using the exact critical temperature $T_c = 2/\ln(\sqrt{2}+1)$, collapse the data for χ' as best as possible onto one curve, plotting $\chi L^{-\gamma/\nu}$ versus $tL^{1/\nu}$, treating γ and ν as fit parameters. What are the best fit values of these exponents? How do they compare to the exact values? What are your greatest sources of error?

2. *Option 1:* Extend your simulation to the q-state Potts model, with $H = -J\sum_{\langle ij\rangle}\delta_{s_i,s_j}$, with $s_i = 1, 2, \cdots, q$. Estimate the critical temperature for $q = 3$ and $q = 10$. Give conclusive evidence that the larger-q model is undergoing a first order phase transition. Examine the finite-size scaling of the peak in the specific heat for $q = 10$: can you determine how it scales with L?

3. *Option 2:* Modify your program to simulate an antiferromagnetic ($J = -1$) on the 2d triangular lattice. Examine the energy, specific heat, and susceptibility for a phase transition. Is there one? Calculate the entropy at very low temperature ($T < 0.1$) by integrating the specific heat:

$$\Delta S = \int_{T_{\text{low}}}^{T_{\text{high}}} \frac{C}{T} dT. \tag{1}$$

What should this integral be, and what do you obtain? Where is the "missing" entropy?

4. *Option 3:* Modify your simulation to the case of anti-periodic boundary conditions in the x direction, i.e. so that the column of horizontal bonds going from $x = L$ to $x = 1$ are antiferromagnetic. In this case, the ordered phase must have a domain wall. Calculate the surface tension of the domain wall as $\epsilon = \left(\langle E\rangle_{\text{APBC}} - \langle E\rangle_{PBC}\right)/L_y$ versus temperature. How much can you understand about its scaling above and below T_c?